

Methyl 4-hydroxy(²H₄)benzoate
362049-51-2 | DTXSID20858080

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 98.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 131</div> <div>Predicted: 98.7</div>	<div>Image not found</div> <div>Methyl 3-hydroxybenzoate</div> <div>Measured: 73.0</div> <div>Predicted: 95.8</div>	<div>Image not found</div> <div>Ethylparaben</div> <div>Measured: 117</div> <div>Predicted: 101</div>
<div>Image not found</div> <div>Ethyl 3-hydroxybenzoate</div> <div>Measured: 74.0</div> <div>Predicted: 93.5</div>		